

Non-Fermi Liquid due to Orbital Fluctuations in Iron Pnictide Superconductors

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We study the influence of quantum fluctuations on the electron self energy in the normal state of iron-pnictide superconductors using a five orbital tight binding model with generalized Hubbard on-site interactions. Within a one-loop treatment, we find that an overdamped collective mode develops at low frequency in channels associated with quasi-1D d_{xz} and d_{yz} bands. When the critical point for the C_4 symmetry broken phase (structural phase transition) is approached, the overdamped collective modes soften, and acquire increased spectral weight, resulting in non-Fermi liquid behavior at the Fermi surface characterized by the frequency dependence of the imaginary part of electron self energy of the form ω^λ , $0 < \lambda < 1$. We argue that this non-Fermi liquid behavior is responsible for the recently observed zero-bias enhancement in the tunneling signal in point contact spectroscopy. A key experimental test of this proposal is the absence of the non-Fermi liquid behaviour in the hole-doped materials. Our result suggests that quantum criticality plays an important role in understanding the normal state properties of iron-pnictide superconductors.

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Introduction – Whether or not the iron pnictide superconductors are strongly correlated materials is hotly debated. Certainly a clean association of non-Fermi liquid behaviour, either experimentally or theoretically, with any part of the phase diagram would suffice to settle this debate. While parallels with the cuprates are suggestive[1–5], they have not resulted in a decisive answer to this problem. In fact, to our knowledge, the possibility of non-Fermi liquid behaviour other than Mott physics[6] has not been discussed to date.

A feature common to the parent and underdoped compounds of the iron pnictide superconductors is the structural phase transition (SPT) from tetragonal to orthorhombic symmetry occurring around 150K[7]. For most members of the 1111 and 122 families, in-plane anisotropy in the resistivity commences near the structural transition, and stripe-like antiferromagnetism develops if the temperature is further lowered. The quasi-particle interference in STM[9] also showed the anisotropic electronic states at very low temperature. Despite the controversy of whether the SPT is induced by magnetic fluctuations as a result of the onset of stripe-like antiferromagnetism[10–14] or if orbital ordering in quasi-1D d_{xz} and d_{yz} bands[15–18] is the efficient cause, the phase below the SPT breaks C_4 symmetry, and quantum fluctuations associated with this phase are nematic in character. A recent measurement of photoexcited quasiparticle relaxation[19] reveals the existence of strong nematic fluctuations up to 200K, well above the SPT temperature. Moreover, in electron-doped Ba(Fe_{1-x}Co_x)₂As₂ (Ba122), an unexpected enhancement of the zero-bias signal[20, 21] in the tunneling signal measured in point contact spectroscopy has been observed at an onset temperature higher than the SPT temperature. The excess conductance appears at temperature around 175K, increasing in magnitude through the structural, antiferromagnetic, and, in materials ex-

hibiting superconductivity, through the superconducting transitions. It is not seen in overdoped Ba122. It is important to study how these strong orbital (nematic) fluctuations affect the physical properties in both the normal and orthorhombic states of the iron pnictide superconductors.

In this Letter, we develop a microscopic theory for the orbital fluctuations and show that they give rise to non-Fermi liquid behaviour. In particular, we find a branch of overdamped collective modes in the scattering channels associated with quasi-1D d_{xz} and d_{yz} bands in the normal state at a temperature higher than the SPT. In the vicinity of the SPT critical point, these overdamped collective modes dominate the low energy physics, resulting in a strong modification of the electron self energy and a breakdown of Fermi-liquid theory even in the symmetric normal state.

RPA theory for electron self energy – While there is no guarantee that non-Fermi liquid behaviour can be captured by a diagrammatic approach of the type employed here, a recent non-perturbative calculation of the electron self-energy in the presence of nematic fluctuations was found to be in full agreement with a perturbative treatment[22]. As the same physics is relevant here, we contend that a perturbative treatment is sufficient to establish our key claim of non-Fermi liquid behaviour from orbital fluctuations. Our starting point is the Hamiltonian $H = H_t + H_I$, where $H_t = \sum_{\vec{k}} H_{\vec{k}}$ is the five-band tight binding model proposed in Ref. [23] which can reproduce correctly the Fermi surfaces of hole α_1, α_2 and electron pockets β_1, β_2 in the unfolded Brillouin zone. The interaction terms are given by H_I

$$H_I = \sum_{ia} U n_{ia\uparrow} n_{ia\downarrow} + \sum_{i,b>a} (U' - \frac{J}{2}) n_a n_b - \sum_{i,b>a} 2J \vec{S}_{ia} \cdot \vec{S}_{ib} + J'(p_{ia} p_{ib}^\dagger + h.c.), \quad (1)$$

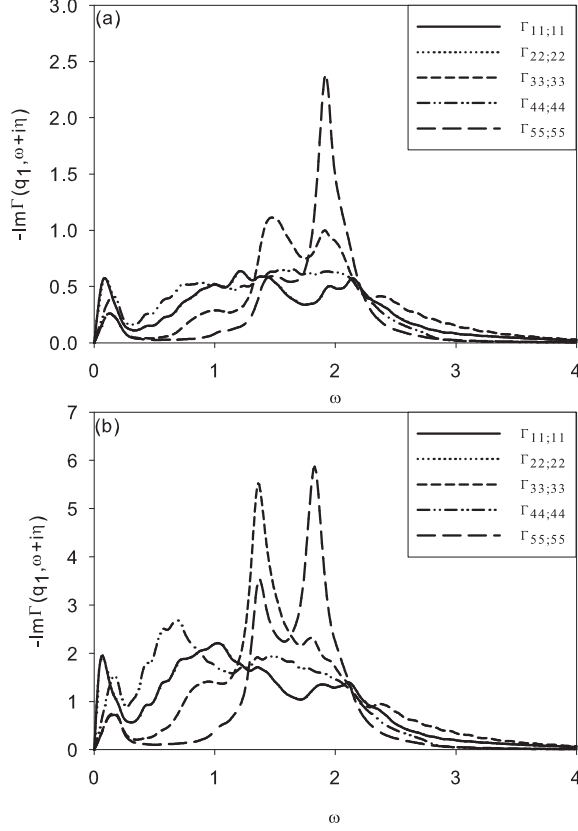


FIG. 1: Spectral functions for effective interactions in intra-orbital channels ($\Gamma_{aa;aa}(\vec{q}, \omega)$) at $\vec{q}_1 = (0.04\pi, 0.04\pi)$ for (a) $U=1.3$ and (b) $U=2.0$. $\Gamma_{11;11}(\vec{q}, \omega) = \Gamma_{22;22}(\vec{q}, \omega)$ for \vec{q} along the diagonal direction as expected, and an overdamped collective mode appearing at low energy in $\Gamma_{11;11}(\vec{q}, \omega)$ ($\Gamma_{22;22}(\vec{q}, \omega)$) can be observed.

where $U' = U - 2J$ and J is the Hund coupling, and a (b) refers to the orbital index, $1 = xz$, $2 = yz$, $3 = xy$, $4 = x^2 - y^2$, and $5 = 3z^2 - r^2$. We introduce a unitary transformation $\hat{U}_{\vec{k}}$ such that $(\hat{U}_{\vec{k}})^\dagger \hat{H}_{\vec{k}} \hat{U}_{\vec{k}} = \text{diag.}[E_{\vec{k},1}, \dots, E_{\vec{k},5}]$, and it is straightforward to obtain the non-interacting response functions,

$$\begin{aligned} & \chi_{ab;cd}^{(0)}(\vec{q}, i\omega_n) \\ &= -\frac{1}{N} \sum_{\vec{k}} \sum_{l,m} (\hat{U}_{\vec{k}+\vec{q}})_{a,l} (\hat{U}_{\vec{k}+\vec{q}})^*_{c,l} (\hat{U}_{\vec{k}})_{d,m} (\hat{U}_{\vec{k}})^*_{b,m} \\ & \times \frac{n_F(E_{\vec{k}+\vec{q},l}) - n_F(E_{\vec{k},m})}{E_{\vec{k}+\vec{q},l} - E_{\vec{k},m} - i\omega_n}, \end{aligned} \quad (2)$$

in the symmetric normal phase, where $\chi_{ab;cd}^{(0)}(\vec{q}, i\omega_n)$ is a 25×25 matrix. The convention on the indices is that in Ref.[23]. Adopting the interaction kernels for the spin-spin (\hat{V}^s) and density-density (\hat{V}^c) fluctuations derived in Ref.[24], we obtain the electron self energy at the

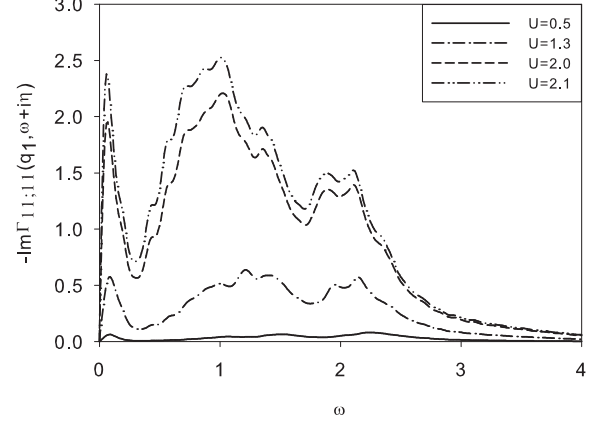


FIG. 2: Spectral functions of effective interactions $\Gamma_{11;11}(\vec{q}_1, \omega)$ at $\vec{q}_1 = (0.04\pi, 0.04\pi)$ for different U . The overdamped collective mode at low energy acquires increased spectral weight as the critical point ($U_c \approx 2.1\text{eV}$ at the temperature we are considering $k_B T = 0.02\text{eV}$) is approached.

random-phase approximation level,

$$\Sigma_{ab}^{\text{orbital}}(\vec{k}, ip_n) = \frac{1}{\beta N} \sum_{\vec{q}} \sum_{ik_m} \hat{\Gamma}_{ai;jd}(\vec{q}, ip_n - ik_m) \hat{G}_{ij}^0(\vec{k} - \vec{q}, ik_m), \quad (3)$$

where ik_m, ip_n are Matsubara frequencies for fermions, $\hat{G}^0(\vec{k}, ip_n) = [ip_n - \hat{H}_t + \mu]^{-1}$ is the bare Green function, and $\hat{\Gamma}_{ab;cd}(\vec{q}, ip_n - ik_m)$ is the effective interaction,

$$\begin{aligned} \hat{\Gamma}(\vec{q}, ip_n - ik_m) &= \frac{1}{2} \{ 3[1 - \hat{V}^s \hat{\chi}_0(\vec{q}, ip_n - ik_m)]^{-1} \hat{V}^s \\ & - [1 + \hat{V}^c \hat{\chi}_0(\vec{q}, ip_n - ik_m)]^{-1} \hat{V}^c \} \end{aligned} \quad (4)$$

within one-loop. Throughout this paper, the temperature is set to be $k_B T = 0.02\text{eV}$ at which the system is in a normal state without any symmetry breaking.

Consider first the spectral functions for the effective interactions $-\text{Im}\hat{\Gamma}(\vec{q}, \omega + i\eta)$ displayed in Fig. 1. As is evident, the spectral functions for the intra-orbital effective interactions $-\text{Im}\Gamma_{aa;aa}(\vec{q}_1, \omega)$ dominate the electron self energy. Also of interest are the spectral functions for momenta \vec{q} along the diagonal direction so that $\Gamma_{11;11}(\vec{q}, \omega) = \Gamma_{22;22}(\vec{q}, \omega)$. It can be seen in Fig. 1 that the spectral functions at low frequency are dominated by an overdamped collective mode in $\Gamma_{11;11}$ ($\Gamma_{22;22}$). When U is tuned to approach the critical point ($U_c \approx 2.1$ at this temperature), this mode gains more spectral weight and moves to even lower energy as shown in Fig. 2.

These overdamped modes, emergent at low frequency and small \vec{q} , resemble the collective modes observed in the *quadrupole density spectral function*[22, 25, 26], that is, the spectral function related to the interactions in the *d*-wave channel in a quantum nematic Fermi fluid. As shown in Ref. [27], in a system containing quasi-1D d_{xz}

and d_{yz} bands, band hybridizations enhance significantly the strength of the interaction in the d -wave channel. As a result, the nematic order in such multiorbital systems is completely **equivalent** to orbital ordering in quasi-1D bands, and the spectral functions due to quantum fluctuations associated with the quasi-1D bands naturally acquire the same properties of quadrupole density spectral function discussed in the context of the quantum nematic fluid mentioned above. It has been shown[22, 25, 26] that these overdamped collective mode could lead to a non-Fermi liquid near the critical region and also in the nematic phase. The reason is that in the vicinity of the nematic critical point, these overdamped collective modes become soft. Electrons scatter strongly with these soft overdamped collective modes, which modifies the electron self energy away from the Fermi liquid behavior in the vicinity of the nematic critical point. In the nematic phase, these overdamped collective modes evolve into Goldstone modes[28] but remain overdamped and dominate the low energy physics. Consequently, the non-Fermi liquid persists in the nematic phase.

It is intriguing to check whether the same physics discussed above occurs in the iron pnictide superconductors since the SPT signals a transition from the symmetric normal phase to a phase breaking C_4 symmetry. We performed a numerical evaluation of Eq. 3. To compute the self energy of the retarded Green function of a single-particle state on the Fermi surface, we need to do one more transformation and also an analytical continuation on Eq. 3 to obtain

$$\Sigma_{\alpha\alpha}^{band}(\vec{k}_F, \omega + i\eta) = (\hat{U}_{\vec{k}_F} \hat{\Sigma}^{orbital}(\vec{k}_F, \omega + i\eta) \hat{U}_{\vec{k}_F}^\dagger)_{\alpha\alpha}, \quad (5)$$

which is the self energy of the electron with momentum \vec{k}_F on the Fermi surface sheet α . Because we study the normal state at finite temperature, $\Sigma_{\alpha\alpha}^{band}(\vec{k}_F, \omega + i\eta)$ contains contributions from both thermal and quantum fluctuations. At low frequency, we can generally write $-\text{Im}\Sigma_{\alpha\alpha}^{band}(\vec{k}_F, \omega + i\eta) \approx a(T) + b(T)\omega^\lambda$ where $a(T), b(T)$ are temperature-dependent constants. A Fermi liquid yields $\lambda = 2$, and $\lambda < 1$ signals a non-Fermi liquid.

To see the frequency dependence more clearly, in Fig. 3 we plot the normalized imaginary part of the self energy defined as

$$\text{Im}\Sigma_{\alpha\alpha}^{nor}(\vec{k}_F, \omega) \equiv \frac{(\text{Im}\Sigma_{\alpha\alpha}^{band}(\vec{k}_F, \omega) - \text{Im}\Sigma_{\alpha\alpha}^{band}(\vec{k}_F, 0))}{\text{Im}\Sigma_{\alpha\alpha}^{band}(\vec{k}_F, 0)} \quad (6)$$

A crossover from Fermi liquid ($\lambda = 2$) to non-Fermi liquid ($\lambda \leq 1$) behaviour can be seen as U is increased to approach the critical point. In the critical region, non-Fermi liquid behavior exists in a large part of the Fermi surface with strong angular dependence of $\text{Im}\Sigma$ as expected due to the critical fluctuations near orbital ordering (now termed nematicity)[25]. As the temperature is lowered, the critical point U_c shifts to a lower value but

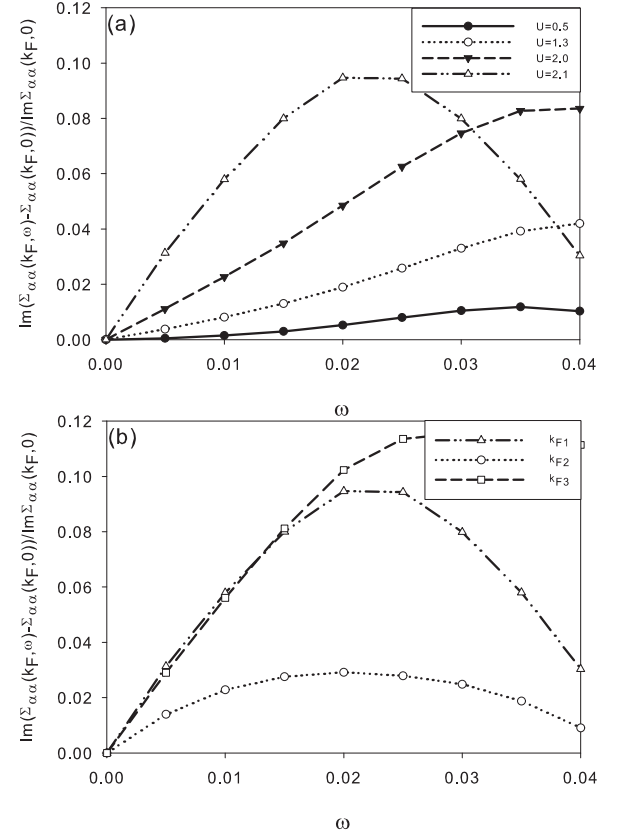


FIG. 3: (a) Normalized self-energy of electron with momentum $\vec{k}_F = (0.12\pi, 0.12\pi)$ on the hole Fermi pocket α_1 for different U . A crossover from Fermi liquid ($\lambda = 2$) to non-Fermi liquid ($\lambda \leq 1$) can be seen as U increases from $U = 0.5$ to critical point $U = 2.1$. (b) Normalized self-energy of electron in the critical region ($U=2.1$) with momenta $\vec{k}_{F1} = (0.12\pi, 0.12\pi)$, $\vec{k}_{F2} = (0.2\pi, 0)$ on hole Fermi pocket α_1 , and $\vec{k}_{F3} = (0.88\pi, 0.16\pi)$ on electron Fermi pocket β_1 .

the non-Fermi liquid behavior remains robust near the critical point. This strongly suggest that this non-Fermi liquid behavior should be observable in iron-pnictide superconductors at a temperature above the SPT and will persist even below the SPT temperature. A sketch of the region in the phase diagram exhibiting the non-Fermi liquid behavior is plotted in Fig. 4.

Experimental Consequences – A direct consequence of non-Fermi liquid behavior is the temperature dependence of the resistivity. It has been pointed out[29], by investigating various iron-pnictide superconductors, that a strong deviation from the Fermi liquid T^2 behavior of resistivity above the SPT temperature would occur if a large anisotropy in in-plane resistivity exists below the SPT temperature. This provides direct evidence for our claim that non-Fermi liquid behaviour is due to orbital fluctuations.

What about the zero-bias anomaly seen in point-

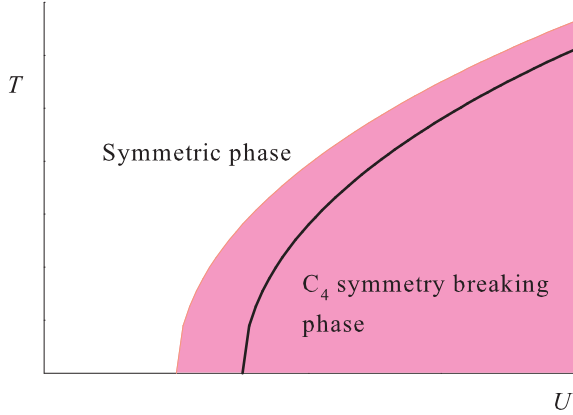


FIG. 4: (Color online) Sketch of regions in the phase diagram showing non-Fermi liquid behavior (colored area). Solid line marks the phase boundary of the transition from symmetric to C_4 symmetry breaking phases.

contact experiments[20, 21] on electron-doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$? Intriguingly, this zero-bias enhancement starts to appear at temperatures roughly 30K higher than the SPT temperature and remains robust well below the SPT temperature. This observation is also consistent with our theory. It has been shown by Lawler *et al.*[22] that the single particle density of states has the form of

$$N^*(\omega) = N^*(0) + B\omega^{2/3} \ln \omega + \dots \quad (7)$$

in the nematic critical region and also in the nematic phase. In fact, $N^*(\omega)$ obtains extra contributions due to the non-Fermi liquid self-energy, giving rise to a cusp at zero frequency and a subsequent decrease as the frequency increases. This provides a direct explanation for the zero-bias enhancement observed in point contact spectroscopy since the conductance dI/dV roughly measures the single particle density of states for small frequency. Moreover, since the form of the single particle density of states is the same up to some mild modifications in the vicinity of the critical point and also in the C_4 symmetry broken phase, the zero-bias enhancement should have a smooth crossover as the SPT temperature is crossed, which in fact has been noticed in the quantum point-contact measurement[20, 21]. We predict that for hole-underdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ which does not have an in-plane resistivity anisotropy[29], the zero-bias enhancement should be either not existent or much weaker than that in electron-doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$.

Conclusion – In this Letter we have presented a theory of non-Fermi liquid in a five-band model with generalized Hubbard on-site interactions for iron pnictide superconductors. At the level of the random-phase approximation, we found a branch of overdamped collective

modes emergent at low frequency in channels associated with quasi-1D d_{xz} and d_{yz} bands, and we have shown that these modes become dominant at low energies near the critical point for C_4 symmetry broken phase, leading to non-Fermi liquid behavior. Our theory indicates that quantum criticality could play an important role in understanding the normal state properties of the iron pnictide superconductors.

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